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CFD phenomenological model of solid–liquid mixing in stirred vessels

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Abstract

Particle migration in a concentrated viscous suspension subjected to a non-homogeneous shear field was computed using a 3D extension of the diffusion model of Phillips et al. [Phillips, R. J., Armstrong, R. C., Brown, R. A., Graham, A. L., & Abott, J. R. (1992). A constitutive equation for concentrated suspensions that accounts for shear-induced particle migration. *Physics of Fluids A*, *4*, 30–40]. The numerical results were compared to experimental data from the literature for simple flows and to our own data in the case of two helical ribbon based mixing systems. It is shown that this type of diffusion model, which was developed to predict the behavior of concentrated suspensions dominated by particle–particle interactions, can predict migration trends but definitely requires additional improvements.

Keywords: Mixing; Particle migration; Concentrated suspensions; CFD; Simulations

1. Introduction

The makedown of viscous suspensions at high solids content is a unit operation involved in the production of coatings, specialty chemicals, drugs and space fuels. This operation is generally carried out in batch or semi-batch mode in stirred vessels. The very viscous nature of the media and the homogeneity requirements for the resulting mixture impede the use of classical impeller mixers. Hence, adapted mixing technologies such as planetary mixers with kneading blades (Zhou, Tanguy, & Dubois, 2000) and multishaft mixers that combine in a single apparatus a high-speed dispersing turbine, a pumping impeller and a wall scraping blade (Tanguy, Bertrand, Thibault, & Galy-Jammou, 2001) are common options. From an industrial perspective, however, these mixers are costly to acquire, operate and maintain.

In the polymer industry, it is well known that viscous mixing is best achieved with close-clearance impellers like helical ribbon impellers. For the makedown of high solids content viscous suspensions, as the level of viscosity induced by the high solids concentration and sometimes by the suspending matrix itself is comparable to that obtained in many polymerization processes, it would be tempting to use helical ribbon impellers. In practice, however, this approach is not used by fear of particle segregation in poorly mixed regions and particle migration under non-uniform shear, which might lead to suspension demixing and therefore mixture quality problems. As an example of industrial impact, shear-induced migration of conductive particles is sometimes responsible for the loss of electrical conductivity in polymer compounds (Jana, 2003).

Since the first observations of particle diffusion under shear deformation by Gadala-Maria and Acrivos (1980), several contributions have led to a better understanding of the hydrodynamic phenomena that induce demixing within concentrated suspensions (Altobelli, Givler, & Fukushima, 1991; Leighton & Acrivos, 1986, 1987a,b). It has been shown in particular that the diffusion is related to the particle collision frequency as well as the variations in the suspension viscosity. In 1992, Phillips, Armstrong, Brown, Graham, and Abott (1992) proposed a conservation equation for the solid phase that includes convective transport, collision-induced diffusion, and viscosity effects. These authors used the Krieger and Dougherty model (Krieger & Dougherty, 1959) to express the variation of the suspension viscosity as a function of the solid volume fraction. They combined this equation with the momentum conservation equation for the continuous phase to investigate the diffusion of

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Nomenclature

a	particle diameter (m)
c	impeller distance to the bottom of the tank
D	impeller diameter
D_T	tank diameter
H	liquid height in tank
K	consistency index (Pa s^n)
K_c	empirical constant
K_η	empirical constant
n	shear-thinning or power-law index
N	rotational speed (rev/s)
N_mig	migration number
p	pressure (Pa)
t	time (s)
T	torque (N m)
V	velocity (m/s)

Greek letters

$\dot{\gamma}$	rate-of-strain tensor (s^{-1})
η	viscosity (Pa s)
ρ	density (kg/m^3)
ϕ	particle concentration (v/v)
ϕ_m	maximum particle concentration (v/v)
Ω	computational domain

concentrated monodisperse suspensions of PMMA (polymethyl methacrylate) particles in silicon oil ($45 < \phi < 55$ vol.%). The particles were non-colloidal ($a = 675$ μm) and neutrally buoyant. Couette and Poiseuille flows were studied. It was shown that for these two 'academic' flows, a concentration gradient was generated in the radial direction. Model results were shown to compare well with experimental particle concentration profiles obtained by nuclear magnetic resonance (NMR).

The phenomenon of particle migration was also modeled in the case of particle resuspension in horizontal ducts, in the laminar and transition regimes (Zhang & Acrivos, 1994). The authors complemented the model of Phillips et al. (1992) with a flux term to account for particle settling and thus make it usable for non-neutrally buoyant particles. Here again, the prediction of the solids concentration was compared with NMR measurements from Altobelli et al. (1991). This study highlighted the effect of the Reynolds number and the suspension concentration on the resuspending mechanism. From a qualitative standpoint, the solid–liquid interface was correctly captured by the numerical model.

Particle migration along solid walls was also investigated (Jana, Kapoor, & Acrivos, 1995). An apparent wall slip velocity coefficient was determined experimentally, and was shown to be insensitive to the shear rate while being rather strongly influenced by the solids content of the suspension.

Finally, a few studies have used the model of Phillips et al. (1992) to simulate particle migration within concentrated suspensions flowing between parallel plates and in the gap of off-centered cylinders. In particular, Fang and Phan-Thien (1995) showed that the model predictions are in very good agreement with the analytical solution of the flow between parallel plates. However, the results on the solid volume fraction in the core of the eccentric cylinder problem has not been validated.

The model of Phillips et al. (1992) is not the only model that can be used to simulate the flow of concentrated suspensions. In a recent paper by Tanguy, Thibault, Ascanio, and Brito-De La Fuente (2006), the performance of the network-of-zone approach (Mann & Hackett, 1988) used in combination with the virtual finite element method (Bertrand, Tanguy, & Thibault, 1997) to analyze the complex flow and suspension mechanisms in a coaxial mixer was investigated. Experiments carried out at lab scale confirmed the validity of the predictions. However, this model could not capture the shear-induced particle migration, and as a result, the agreement between the numerical and the experiments in the intensely sheared zones was unsatisfactory.

In all the above approaches, the solid phase is considered as a continuum. However, it is possible to use direct numerical simulation to describe the motion of each individual particle in the liquid phase. The strategy consists of solving the Navier-Stokes equations in the liquid phase while taking into account the presence of the particles through its physical properties and their motion through Newton's second law of motion for each particle (Glowinski, Pan, & Perieux, 1994; Hu, 1996; Hu, Joseph, & Crochet, 1992; Maury & Glowinski, 1997). This approach allows for particle–particle and particle–fluid interactions within the suspension to be modeled in a physically correct manner. In practice, due to computer limitations, the number of particles is limited to a few thousand, whereas in a typical mixing application this number is several orders of magnitude larger.

The objective of the present study is to assess the accuracy of the model proposed by Phillips et al. (1992) and augmented as per Zhang and Acrivos (1994), to capture the particle suspending phenomenon and particle migration in solid–liquid mixing. We call this model the shear-induced migration model (SIMM). Three mixing systems will be considered: a propeller and two helical ribbon geometries. Since these mixing systems lead to complex three-dimensional flows, there are no analytical solutions to the corresponding flow fields so that experimental results will be used for validation. The present work can be considered as a real, asymmetrical three-dimensional application of the model of Phillips et al. (1992) to a mixing situation. To our knowledge, there does not exist a similar application in the literature, the closest being the one presented by Subia, Ingber, Mondy, Altobelli, and Graham (1998).

2. Experimental systems

The first experimental set-up (Fig. 1) consists of a small reservoir (glass beaker) with diameter $D_\mathrm{T} = 7.2$ cm and height $H = 6.5$, and a down-pumping marine propeller with diameter $D = 1.8$ cm that provides agitation. The propeller is located at a distance $c = 2.6$ cm from the bottom.

The investigation of the particle motion inside this mixer involved a Newtonian solution of corn syrup with a viscosity of 1.05 Pa s and a density of 1360 kg/m^3. The particles were red Ballotini glass beads. The spherical beads had a uniform diame-